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MONTE CARLO SURFACE FLUX TALLIES

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ABSTRACT

Particle fluxes on surfaces are difficult to calculate with Monte Carlo codes because the score requires a division by the surface-crossing angle cosine, and grazing angles lead to inaccuracies. We revisit the standard practice of dividing by half of a cosine "cutoff" for particles whose surface-crossing cosines are below the cutoff. The theory behind this approximation is sound, but the application of the theory to all possible situations does not account for two implicit assumptions: 1) the grazing band must be symmetric about 0, and 2) a single linear expansion for the angular flux must be applied in the entire grazing band. These assumptions are violated in common circumstances; for example, for separate in-going and out-going flux tallies on internal surfaces, and for out-going flux tallies on external surfaces. In some situations, dividing by two-thirds of the cosine cutoff is more appropriate. If users were able to control both the cosine cutoff and the substitute value, they could use these parameters to make accurate surface flux tallies. The procedure is demonstrated in a test problem in which Monte Carlo surface fluxes in cosine bins are converted to angular fluxes and compared with the results of a discrete ordinates calculation.

Key Words: Monte Carlo surface flux tallies.

1. INTRODUCTION

The total particle flux on a surface is calculated in Monte Carlo codes by scoring the weight of each particle crossing the surface divided by the cosine of the angle between the particle trajectory and the surface normal [1, 2]. When a particle grazes the surface, the cosine of the surface-crossing angle is small, and the particle's score can be huge, leading to infinite variances and tallies that may have difficulty converging. In some practical situations, both the surface flux tally mean and its variance may be inaccurate.

To circumvent this problem, Clark [1] recommended "exclud[ing] grazing fluxes from the stochastic estimate," replacing them with "an independent estimate of the contribution from grazing angles." Clark's main concern was to overcome the infinite variance that is associated with grazing. In this paper, we are concerned with the accuracy of the fix that is used, not with the accuracy or finiteness of the variance.

The standard estimate of the contribution from grazing angles, which can be inferred from Clark's theoretical analysis, is as follows. Let μ represent the cosine of the surface-crossing angle. Let $0 \le |\mu| \le \varepsilon$, where ε is small, represent the "grazing band" (in the language of Ref. 1). Then the prescription is: When $|\mu| > \varepsilon$, score $1/|\mu|$ as normal, but when $|\mu| \le \varepsilon$, score $2/\varepsilon$. In other words, use $2/\varepsilon$ as an estimate of the expected value of $1/|\mu|$ for grazing angles, defined as angles for which $|\mu|$ is smaller than ε. In the MCNP5 general-purpose Monte Carlo code [3], for example, whenever $|\mu|$ is less than $\varepsilon = 0.1$, $2/\varepsilon = 20$ is scored instead. In Ref. 2, $\varepsilon = 0.01$ is suggested.

For years, the standard approximation has been considered accurate if the angular flux on the surface is isotropic or linearly anisotropic. This assumption is due to Clark [1], who expanded the surface flux as $\phi(\mu) = g_0 + g_1\mu$. Recently [4], however, the accuracy of the standard approximation was found to require a very isotropic flux on external surfaces, not a linearly anisotropic flux. In this paper, we quantify the phrase "very isotropic." We also generalize the results of Ref. 4 to certain cases of internal surfaces.

2. ASSUMPTIONS OF THE STANDARD APPROXIMATION

Let $J(\mu)$ represent the angular surface-crossing rate (or angle-dependent current) on a fixed surface. Then the expected (average) value of $1/\mu$, $\overline{1/\mu}$, for particles sampled on the surface from the function $J(\mu)$ in the range $[-\varepsilon_1, \varepsilon_2]$ is

$$\overline{1/\mu} = \frac{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu \frac{J(\mu)}{|\mu|}}{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu J(\mu)}. \tag{1}$$

The angular flux $\phi(\mu)$ on the surface is the current $J(\mu)$ divided by the surface crossing cosine $|\mu|$, or the integrand in the numerator of Eq. (1) [2]. The integrand in the denominator of Eq. (1) is identified as $|\mu|\phi(\mu)$. Thus Eq. (1) becomes

$$\overline{1/\mu} = \frac{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu \phi(\mu)}{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu |\mu| \phi(\mu)}. \tag{2}$$

Following Clark, we expand the angular flux in a power series of μ,

$$\phi(\mu) = \sum_{i=0}^{\infty} g_i \mu^i, \tag{3}$$

and retain only the first two terms in the expansion; using the result in Eq. (2) yields

$$\overline{1/\mu} = \frac{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu (g_0 + g_1\mu)}{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu (g_0|\mu| + g_1\mu|\mu|)}. \tag{4}$$

At this point we adopt the notation of Ref. 4. The cutoff below which $|\mu|$ is considered a grazing cosine is μ_{cut}. The reciprocal of $\overline{1/\mu}$ is the appropriate substitute cosine divisor to use when $|\mu| < \mu_{cut}$; thus, $\mu_{sub} \equiv 1/\overline{1/\mu}$. Equation (4) becomes

$$\mu_{sub} = \frac{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu (g_0|\mu| + g_1\mu|\mu|)}{\int_{-\varepsilon_1}^{\varepsilon_2} d\mu (g_0 + g_1\mu)}. \tag{5}$$

The standard approximation is based on Eq. (5), but it has two implicit assumptions.

2.1. The Grazing Angle Integral is Symmetric

The standard approximation assumes that the grazing range integral over which the expected value is estimated is symmetric about 0; in other words, $\varepsilon_1 = \varepsilon_2 = \mu_{cut}$ in Eq. (5). If this is the case, then the g_1 term integrates to zero in both the denominator and the numerator of Eq. (5), and the g_0 term simplifies nicely, leaving the standard approximation, which in the present notation is

$$\mu_{sub} = \mu_{cut}/2. \tag{6}$$

In at least two production Monte Carlo codes, MCNPX [5] and Mercury [6], μ_{cut} is hard-coded but users are allowed to use cosine bins for surface-flux tallies. Consider a bin whose boundaries $[\varepsilon_1, \varepsilon_2]$ are both positive but within the grazing band. Then the appropriate substitute value is

$$\mu_{sub} = \frac{\int_{\varepsilon_1}^{\varepsilon_2} d\mu (g_0|\mu| + g_1\mu|\mu|)}{\int_{\varepsilon_1}^{\varepsilon_2} d\mu (g_0 + g_1\mu)} = \frac{\frac{1}{2}\frac{g_0}{g_1}(\varepsilon_2^2 - \varepsilon_1^2) + \frac{1}{3}(\varepsilon_2^3 - \varepsilon_1^3)}{\frac{g_0}{g_1}(\varepsilon_2 - \varepsilon_1) + \frac{1}{2}(\varepsilon_2^2 - \varepsilon_1^2)}. \tag{7}$$

If the bin boundaries $[-\varepsilon_1, -\varepsilon_2]$ are both negative but within the grazing band, then the appropriate substitute value is

$$\mu_{sub} = \frac{\frac{1}{2}\frac{g_0}{g_1}(\varepsilon_2^2 - \varepsilon_1^2) - \frac{1}{3}(\varepsilon_2^3 - \varepsilon_1^3)}{\frac{g_0}{g_1}(\varepsilon_2 - \varepsilon_1) - \frac{1}{2}(\varepsilon_2^2 - \varepsilon_1^2)}. \tag{8}$$

Finally, if the lower bin boundary is $-\varepsilon_1$ (negative) and the upper bin boundary is ε_2 (positive) and both of these are within the grazing band, then the appropriate substitute value is

$$\mu_{sub} = \frac{\frac{1}{2}\frac{g_0}{g_1}(\varepsilon_2^2 + \varepsilon_1^2) + \frac{1}{3}(\varepsilon_2^3 - \varepsilon_1^3)}{\frac{g_0}{g_1}(\varepsilon_2 + \varepsilon_1) + \frac{1}{2}(\varepsilon_2^2 - \varepsilon_1^2)}. \tag{9}$$

In this last case, setting $\varepsilon_1 = \varepsilon_2 = \mu_{cut}$ makes the integral symmetric and recovers the standard approximation of Eq. (6).

The standard approximation is designed to estimate the entire flux integral in the grazing band, so obviously it will not be correct to use it to estimate the integral in some portion of the grazing band, not even a symmetric portion in which $\varepsilon_1 = \varepsilon_2 \neq \mu_{cut}$. In general, the right sides of Eqs. (7), (8), and (9) will not be equal to $\mu_{cut}/2$ and the standard approximation does not apply, even if the flux is purely isotropic ($g_1 = 0$). This observation is not new or novel but it is worth repeating and including in the code manuals when user-defined cosine bins are allowed.

On the other hand, suppose it is desired to compute the flux in the half-plane, $0 \le \mu \le 1$ or $-1 \le \mu \le 0$. In the positive-μ case, the lower bin boundary ε_1 goes to zero in Eq. (7) or (9), the upper bin boundary becomes μ_{cut}, and the appropriate substitute value in the grazing range is

$$\frac{\mu_{sub}}{\mu_{cut}} = \frac{\frac{1}{2}\frac{g_0}{g_1} + \frac{1}{3}\mu_{cut}}{\frac{g_0}{g_1} + \frac{1}{2}\mu_{cut}}. \tag{10}$$

In the negative-μ case, the upper bin boundary ε_2 goes to zero in Eq. (8) or (9), the lower bin boundary becomes $-\mu_{cut}$ (negative), and the appropriate substitute value in the grazing range is

$$\frac{\mu_{sub}}{\mu_{cut}} = \frac{\frac{1}{2}\frac{g_0}{g_1} - \frac{1}{3}\mu_{cut}}{\frac{g_0}{g_1} - \frac{1}{2}\mu_{cut}}. \tag{11}$$

In both cases, if the flux is purely isotropic ($g_1 = 0$), the standard approximation of Eq. (6) is obtained. However, if the flux is purely linear ($g_0 = 0$), the appropriate substitute value is

$$\mu_{sub} = 2\mu_{cut}/3. \tag{12}$$

This equation was also derived in Ref. 4. As Clark [1] notes, g_0 must be non-zero within a medium, but g_1 must be non-zero at an external boundary (although a special case having $g_1 = 0$ on an external boundary can probably be concocted). Thus, Eq. (12) will apply only for external boundaries. However, on any surface, if the flux has both isotropic and linear components (g_0

and g_1 both not zero), what is the appropriate substitute value? This question will be addressed in Sec. 3.

2.2. The Linear Flux Expansion is Accurate in the Entire Grazing Range

The standard approximation naturally assumes that coefficients of the angular flux linear expansion (g_0 and g_1) are constant over the grazing range; i.e., simply that the assumed flux expansion is accurate. Even if the integral in the grazing range is symmetric about 0, in accordance with the assumption of Sec. 2.1, the estimated expected value of $\overline{1/\mu}$ will be wrong if the assumed expansion is not appropriate. This assumption is obvious, yet it is routinely violated.

Suppose the flux satisfies $\phi(\mu) = g_0 + g_{1,L}\mu$ for $-\mu_{cut} \le \mu \le 0$ and $\phi(\mu) = g_0 + g_{1,R}\mu$ for $0 \le \mu \le \mu_{cut}$. This situation is depicted in Fig. 1. Outside the grazing range, there is curvature, but inside the grazing range, the flux is linear with μ. The appropriate substitute value to apply to the entire grazing range $[-\mu_{cut}, \mu_{cut}]$ is

$$\mu_{sub} = \frac{\int_{-\mu_{cut}}^{\mu_{cut}} d\mu(g_0|\mu| + g_1\mu|\mu|)}{\int_{-\mu_{cut}}^{\mu_{cut}} d\mu(g_0 + g_1\mu)} = \frac{-\int_{-\mu_{cut}}^{0} d\mu(g_0\mu + g_{1,L}\mu^2) + \int_{0}^{\mu_{cut}} d\mu(g_0\mu + g_{1,R}\mu^2)}{\int_{-\mu_{cut}}^{0} d\mu(g_0 + g_{1,L}\mu) + \int_{0}^{\mu_{cut}} d\mu(g_0 + g_{1,R}\mu)}, \tag{13}$$

or

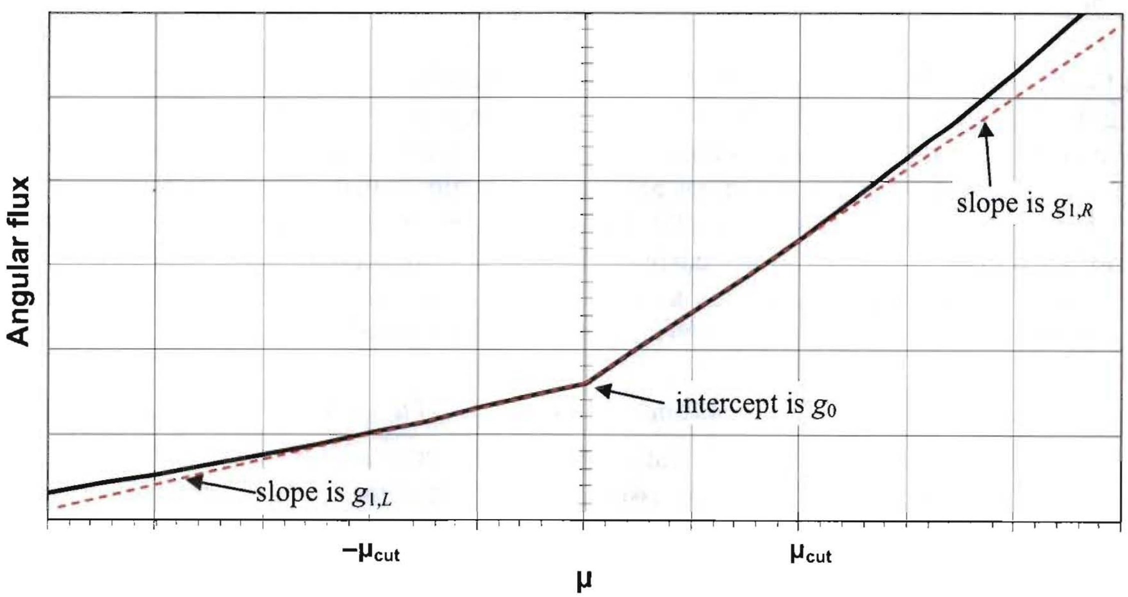

Figure 1. The angular flux on an arbitrary internal interface.

$$\frac{\mu_{sub}}{\mu_{cut}} = \frac{g_0 + \frac{1}{3}\mu_{cut}(g_{1,R} - g_{1,L})}{2g_0 + \frac{1}{2}\mu_{cut}(g_{1,R} - g_{1,L})}. \tag{14}$$

The standard approximation $\mu_{sub}/\mu_{cut} = ½$ assumes $g_{1,R} \approx g_{1,L}$. If the two slopes are too different, the standard approximation will be inaccurate, especially if μ_{cut} is large or the isotropic component g_0 is small.

For the flux on an exterior surface, when there is no incoming current, one of the g_1 coefficients is 0, and the angular flux may be discontinuous across $\mu = 0$ (dropping from a finite value to 0). In this case the grazing range integral limits of $[-\mu_{cut}, \mu_{cut}]$ are inappropriate and the requirement for satisfying this assumption is not valid. Equation (14) does not then apply.

If the flux is zero for $-1 \le \mu \le 0$, then the problem corresponds to computing the flux in the half-plane $0 \le \mu \le 1$ from Sec. 2.1. The appropriate substitute value for the grazing range is given by Eq. (10). Likewise, if the flux is zero for $0 \le \mu \le 1$, the problem corresponds to computing the flux in the half-plane $-1 \le \mu \le 0$ from Sec. 2.1, and the appropriate substitute value for the grazing range is given by Eq. (11).

Thus, on an external surface, where the flux might become very small at $\mu = 0$ ($g_0 \approx 0$) but larger at $\mu = \pm\, \mu_{cut}$ ($\pm g_1 > 0$; the plus or minus depends on the coordinate system as well as the orientation of the surface), the standard approximation might not apply. It requires a more isotropic flux on external surfaces than on internal surfaces.

2.3. Summary

The theory behind avoiding infinite variances and instability in Monte Carlo surface-flux tallies using the expected value of the reciprocal of the grazing surface-crossing cosine is sound. The application of the theory to generate Eq. (6) and apply it uniformly in all cases did not properly account for two situations. First, it has always been assumed that the grazing range would contribute only a small amount to a total scalar flux integral on the surface; the notion that users would be allowed to input arbitrary cosine bins has not been accounted for. Second, the notion that a one-way flux (e.g., on an external surface) violates the requirement that the grazing range integral limits be symmetric about 0 has not ever been identified.

Equations (10) and (11) give the appropriate value of μ_{sub}/μ_{cut} whenever the flux is one-sided, either because of user-defined cosine bin boundaries or because of physical circumstances (e.g., a vacuum boundary). These equations assume that the minimum possible crossing cosine (absolute value) is zero (see Ref. 4 for more on this issue) and that one of the cosine bin boundaries is zero.

If g_0 and g_1 are both not zero, then what is a user to do?

3. AN ACCURATE ESTIMATE OF THE EXPECTED VALUE

As shown in Sec. 2, μ_{sub}, the expected value of the reciprocal of the grazing angle cosine, depends on the coefficients of the linear expansion and on the cosine cutoff.

If the coordinate system is such that particles escape through an exterior surface in the negative-μ direction, such as through the bottom of a cylinder, then normally g_1 would be negative on that surface for $-\mu_{cut} \le \mu \le 0$. Special cases may be set up to violate this condition. However, if g_1 is negative in Eq. (11), then substitute $-|g_1|$ for g_1 and see that Eq. (11) becomes Eq. (10) in this case. Thus, normally, but perhaps not always, Eq. (10) will be the one to apply on exterior surfaces.

Figure 2 is a plot of Eq. (10), showing μ_{sub}/μ_{cut} as a function of g_0/g_1 and μ_{cut}. There is a broad flat region where $\mu_{sub}/\mu_{cut} = \frac{1}{2}$, there is a narrow transition region, and there is a broad flat region where $\mu_{sub}/\mu_{cut} = \frac{2}{3}$. Small values of μ_{cut} and large values of g_0 relative to g_1 (more

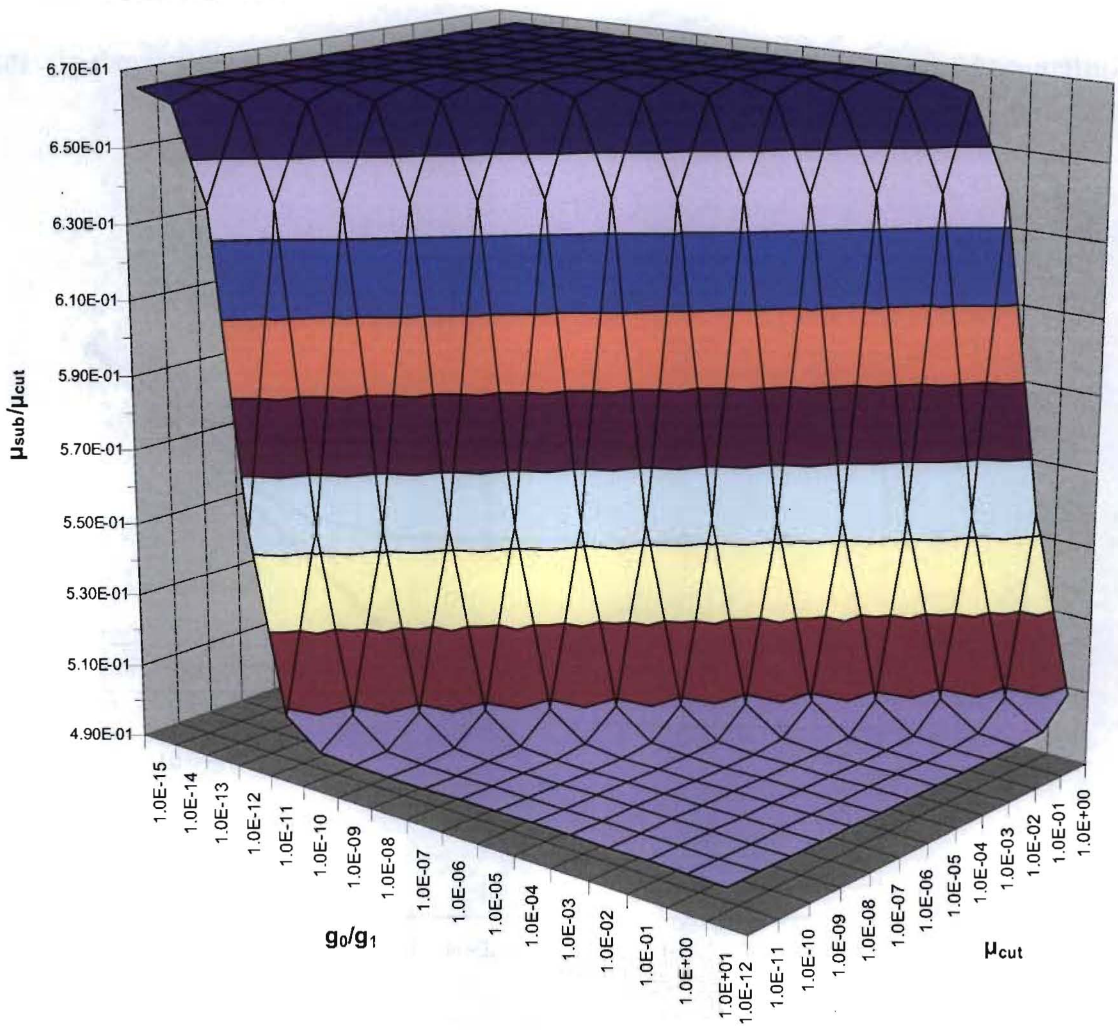

Figure 2. μ_{sub}/μ_{cut} on an exterior surface; from Eq. (10).

isotropy) tend to lead to the standard approximation, $\mu_{sub}/\mu_{cut} = \frac{1}{2}$. On internal surfaces, given the assumptions of Sec. 2, *any* value of g_1 leads to the standard approximation. On exterior surfaces, more isotropy is required, but just how much more depends on the assumed grazing range, or μ_{cut}.

Another way to picture μ_{sub}/μ_{cut} is to plot the angular flux itself as a function of μ. This is done in Fig. 3 for different values of the ratio g_0/g_1, fixing $g_1 = 1$ as an example. Figure 3 shows that there is always some cosine μ below which the flux is approximately constant with μ (on a log-log scale).

Together, Figs. 2 and 3 suggest one approach to the problem of choosing the right value of μ_{sub}/μ_{cut}: Always use the standard value $\mu_{sub}/\mu_{cut} = \frac{1}{2}$, but try to set μ_{cut} to a value below which the flux is approximately constant with μ. That will be the grazing region in which $\mu_{sub}/\mu_{cut} = \frac{1}{2}$ is appropriate. For example, in Fig. 3, the cosine cutoff should be $\sim\frac{1}{10}$ of g_0/g_1. This prescription will be slightly modified in Sec. 4.

The difference between the correct value of μ_{sub}/μ_{cut} for any problem and the standard value of ½ may be quantified by defining f as

$$f \equiv \frac{g_0/g_1}{\mu_{cut}}. \tag{15}$$

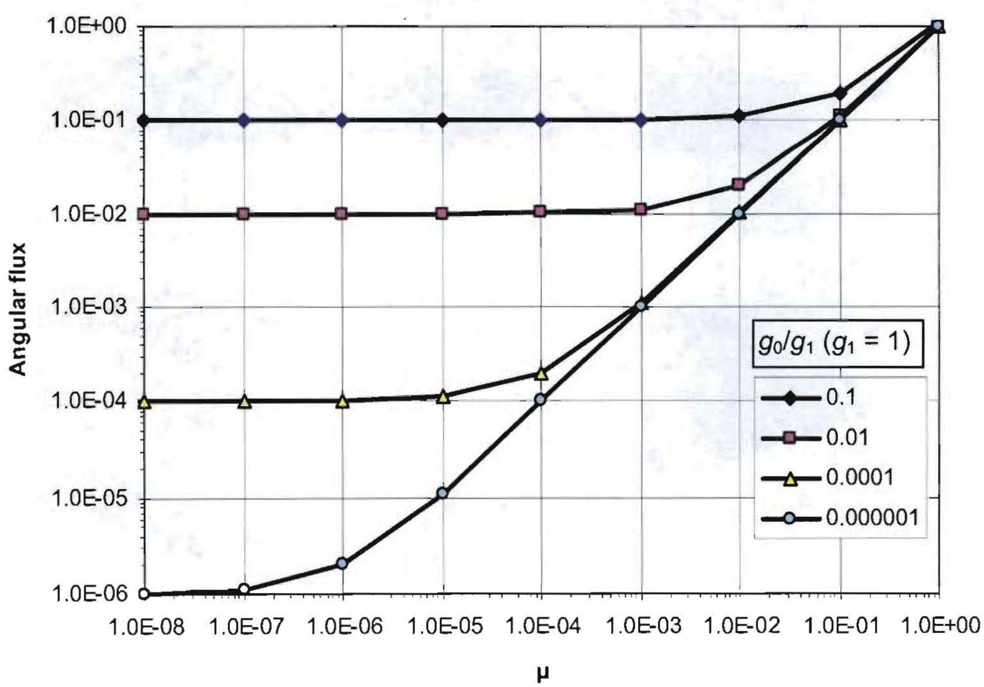

Figure 3. Angular flux assuming a linear form with different values of g_0/g_1, with $g_1 = 1$.

Using this ratio in Eq. (10) yields

$$\frac{\mu_{sub}}{\mu_{cut}} = \frac{\frac{1}{2}f + \frac{1}{3}}{f + \frac{1}{2}}. \tag{16}$$

Now define R_μ to be the relative difference between μ_{sub}/μ_{cut} as given by Eq. (10) [and Eq. (16)] and the desired value of $\mu_{sub}/\mu_{cut} = ½$:

$$R_\mu \equiv \frac{\mu_{sub}/\mu_{cut} - ½}{½}. \tag{17}$$

From Eq. (17), using $½(R_\mu + 1)$ for μ_{sub}/μ_{cut} on the left side of Eq. (16) and solving for R_μ yields

$$R_\mu = \frac{1}{6f+3}. \tag{18}$$

Equation (18), the difference between the correct value of μ_{sub}/μ_{cut} and the standard value of ½, is plotted in Fig. 4. Regardless of the value of g_0/g_1, the standard value becomes more correct as μ_{cut} becomes smaller. Regardless of the value of μ_{cut}, the standard value becomes more correct as the flux gets more isotropic (g_0 increases relative to g_1). Figure 2 shows these effects as well, but Fig. 4 quantifies them.

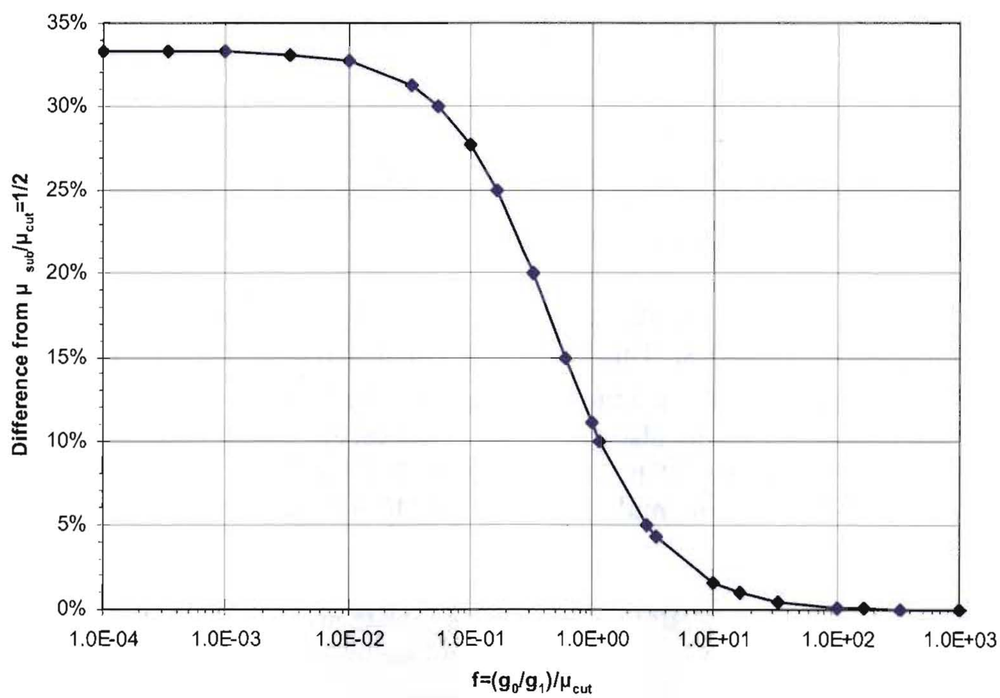

Figure 4. Errors associated with the standard approximation.

What is the error in the estimated grazing range flux associated with using the standard value of μ_{sub}/μ_{cut}? The true grazing range flux ϕ_T is the approximated flux ϕ_A corrected by multiplying by the expected value $\mu_{sub}/\mu_{cut} = ½$ that was applied in the approximation and dividing by the true expected value of μ_{sub}/μ_{cut} from Eq. (16):

$$\phi_T = \phi_A \frac{1}{2} \frac{f + \frac{1}{2}}{\frac{1}{2} f + \frac{1}{3}} = \phi_A \frac{f + \frac{1}{2}}{f + \frac{2}{3}}. \tag{19}$$

Now defining R_ϕ as the difference between ϕ_A and ϕ_T relative to ϕ_T yields

$$R_\phi \equiv \frac{\phi_A - \phi_T}{\phi_T} = \frac{1}{6f + 3}. \tag{20}$$

Comparing Eq. (20) with Eq. (18), $R_\phi = R_\mu$; errors in the value of μ_{sub}/μ_{cut} lead to the same errors in the integrated flux in the grazing range. Thus, the maximum error in the integrated grazing flux is 33%. If the total integrated surface flux is desired and the grazing range flux is only a small fraction of the total, then this error may be negligible. If the grazing range flux itself is of interest, then errors are more important. Of course, if the "true expected value of μ_{sub}/μ_{cut}" is an approximation, as it will be in the next section, then ϕ_T of Eq. (19) is only an estimate of the exact value of the flux in the grazing range.

4. NUMERICAL EXAMPLES

The test problem in this section is a one-dimensional sphere containing a solid ball of ^{235}U at a mass density of 18.74 g/cm^3 surrounded by a shell of ^{12}C at a mass density of 2.1 g/cm^3. The radius of the ^{235}U ball is 6 cm and the outer radius of the ^{12}C shell is 16 cm. The problem is a k_{eff} calculation but for the purpose of demonstrating issues associated with surface-flux tallies it could just as easily be a fixed-source problem.

Calculations were done with a preliminary version of MCNP [3] version 6 [7], which allows cosine bins on surface flux tallies. This version was modified to accept μ_{sub} and μ_{cut} as user inputs. The MCNP calculations used the 30-group MENDF5 cross-section library because, for comparison, the calculations were also done with PARTISN [8] using S_{128} quadrature, P_4 scattering, and the 30-group MENDF5 cross sections. PARTISN fluxes were normalized by dividing by the PARTISN k_{eff} and multiplying by the MCNP k_{eff}. Monte Carlo results are given with 1σ error bars.

The method used to convert MCNP fluxes in cosine bins to angular fluxes for comparison with PARTISN was as follows. First, the cosine bins were set up to correspond with PARTISN S_N ordinates. The smallest bin boundary of -1 was assumed. The next bin boundary was the average of the two smallest discrete ordinates, the next was the average of the next two, and so on, until the average of the two largest ordinates was used. Then the largest bin boundary was set to 1. This procedure gives one tally bin corresponding to each ordinate. The angular flux in each bin was the flux in that bin divided by the weight associated with the corresponding ordinate in the S_N quadrature set. As will be seen, this method worked very well except for $\mu = \pm 1$. Any summing of angular fluxes in quadrature requires multiplication by the S_N weight; in this case, the MCNP fluxes were used directly.

4.1. Internal Surface

The angular flux on the uranium/carbon interface is shown in Fig. 5. In this figure the MCNP calculation was "dumb," using the code's default value of 0.1 for μ_{cut} and $\mu_{sub}/\mu_{cut} = \frac{1}{2}$. Obviously, fluxes within the grazing range are badly calculated; the theory does not allow the code defaults, which can not presently be changed, to be used in this manner. (Figure 5 shows the trouble that the cosine-bin-flux-to-angular-flux conversion method has at the two edge bins corresponding to $\mu = \pm 1$.)

Table I shows the MCNP value for the integrated flux in the grazing range using different values for μ_{cut} but always $\mu_{sub}/\mu_{cut} = \frac{1}{2}$. These values are compared with reference fluxes obtained from MCNP tallies with no grazing approximation (the tallies passed the statistical convergence tests). The values agree well for the left region ($-\mu_{cut} \le \mu \le 0$) but only moderately well for the right region ($0 \le \mu \le \mu_{cut}$) and the combination ($-\mu_{cut} \le \mu \le \mu_{cut}$).

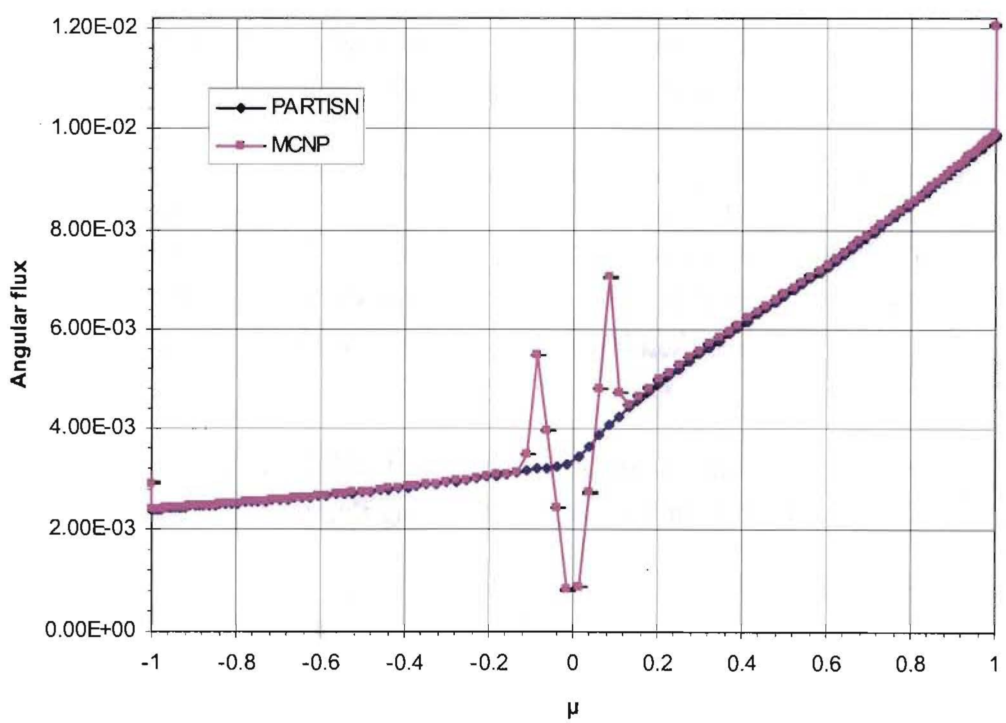

Figure 5. Angular flux on the uranium/carbon interface.

Table I. Effect of the wrong substitute value on the internal interface grazing flux.

Region	μ_{cut}	Flux in the Grazing Range		Difference	μ_{sub}/μ_{cut} Should Be[b]	MCNP Should Be[c]	Difference Should Be
		Reference[a]	MCNP				
Left	**0.097629**	1.599E-04 ± 0.18%	1.586E-04 ± 0.09%	−0.828%	0.4959	1.599E-04	−0.011%
	0.073273	1.208E-04 ± 0.24%	1.201E-04± 0.12%	−0.586%	0.4970	1.208E-04	0.024%
	0.048873	8.105E-05 ± 0.35%	8.076E-05± 0.18%	−0.360%	0.4980	8.109E-05	0.045%
	0.024444	4.082E-05 ± 0.65%	4.081E-05± 0.36%	−0.024%	0.4990	4.089E-05	0.178%
Right	**0.097629**	1.860E-04 ± 0.16%	1.931E-04± 0.08%	3.817%	0.5197	1.857E-04	−0.117%
	0.073273	1.357E-04 ± 0.22%	1.399E-04± 0.11%	3.072%	0.5152	1.357E-04	0.026%
	0.048873	8.774E-05 ± 0.32%	8.964E-05± 0.17%	2.166%	0.5105	8.780E-05	0.069%
	0.024444	4.251E-05 ± 0.63%	4.308E-05± 0.35%	1.342%	0.5054	4.262E-05	0.257%
Comb.	**0.097629**	3.458E-04 ± 0.17%	3.516E-04± 0.08%	1.669%	0.5087	3.456E-04	−0.068%
	0.073273	2.565E-04 ± 0.22%	2.599E-04± 0.11%	1.350%	0.5066	2.565E-04	0.028%
	0.048873	1.688E-04 ± 0.33%	1.704E-04± 0.17%	0.953%	0.5045	1.689E-04	0.059%
	0.024444	8.332E-05 ± 0.64%	8.388E-05± 0.34%	0.673%	0.5023	8.350E-05	0.219%

[a] From MCNP tallies with no grazing approximation.
[b] Equation (11) is used in the left region, Eq. (10) is used in the right, and Eq. (14) is used for the combination.
[c] This column is an approximation of ϕ_T, obtained by multiplying the MCNP column (which is ϕ_A) by ½ and dividing the result by the value that μ_{sub}/μ_{cut} should be.

Linearly fitting the two PARTISN points on each side of $\mu = 0$, the linear flux expansion coefficients are $g_0 = 3.337 \times 10^{-3}$, $g_{1,L} = 1.636 \times 10^{-3}$, and $g_{1,R} = 9.158 \times 10^{-3}$. These values can be used in the equations of Secs. 2 and 3 to estimate what μ_{sub}/μ_{cut} should be as a function of μ_{cut}. Table I shows these estimates for each case and also shows what the MCNP result would be if the updated μ_{sub}/μ_{cut} were used instead of ½ , and it shows what the difference from the reference value would be.

Except for one point (the smallest value of μ_{cut} on the left side), a better value of μ_{sub}/μ_{cut} would yield dramatically better results for the integrated grazing flux than the standard value.

4.2. External Surface

This was the same problem used in the previous section, except here we examine the angular flux on the exterior surface. This is plotted in Fig. 6. Again, the MCNP calculation was "dumb," using the code's default value of 0.1 for μ_{cut} and $\mu_{sub}/\mu_{cut} = \frac{1}{2}$, and fluxes within the grazing range are badly calculated. (Again, Fig. 6 shows the trouble that the cosine-bin-flux-to-

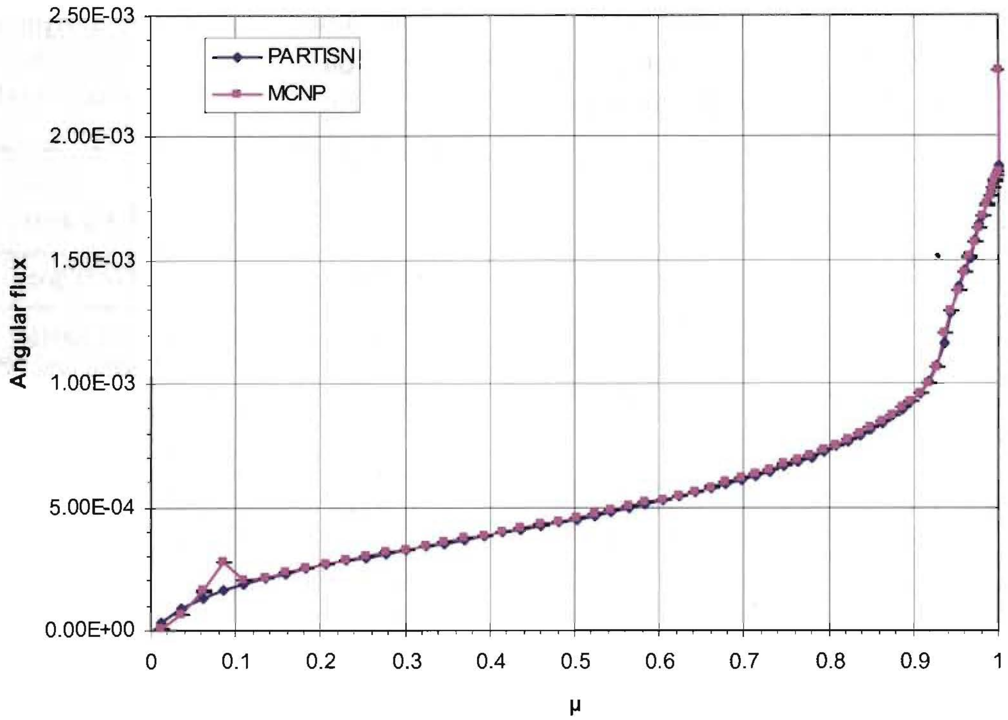

Figure 6. Angular flux on the exterior surface.

angular-flux conversion method has at the edge bin corresponding to $\mu = 1$. Note that this is an artifact of dividing by the S_N weight. When fluxes are summed for the total later in this section, the large difference in this bin will not play a role.)

Linearly fitting the two PARTISN points closest to $\mu = 0$, the linear flux expansion coefficients are $g_0 = 4.562 \times 10^{-6}$ and $g_1 = 2.231 \times 10^{-3}$. This is clearly a case where the isotropic component is essentially 0 and any gradient is large in comparison. Using Eq. (10), the appropriate value of μ_{sub}/μ_{cut} would be $1.980/3 \approx 2/3$ when μ_{cut} is the default value, 0.1. However, as Fig. 6 shows, the flux in the grazing range defined by $\mu_{cut} = 0.1$ is not linear with μ; it is quadratic. Quadratically fitting the four PARTISN points closest to $\mu = 0$, the expansion coefficients are $g_0 = 1.275 \times 10^{-6}$, $g_1 = 2.628 \times 10^{-3}$, and $g_2 = -8.932 \times 10^{-3}$. Keeping three terms in the expansion of Eq. (6), Eq. (10) becomes

$$\frac{\mu_{sub}}{\mu_{cut}} = \frac{\frac{1}{2}g_0 + \frac{1}{3}g_1\mu_{cut} + \frac{1}{4}g_2\mu_{cut}^2}{g_0 + \frac{1}{2}g_1\mu_{cut} + \frac{1}{3}g_2\mu_{cut}^2}. \tag{21}$$

The appropriate values of μ_{sub}/μ_{cut} using Eqs. (10) and (21) are compared in Table II.

What are the consequences of using $\mu_{sub}/\mu_{cut} = \frac{1}{2}$ instead of the correct value? Figure 7 is a plot of the total integrated flux on the surface as a function of the grazing cosine cutoff μ_{cut}. The MCNP results use $\mu_{sub}/\mu_{cut} = \frac{1}{2}$, $\mu_{sub}/\mu_{cut} = \frac{2}{3}$, or Eq. (21) over the whole range.

Table II. Appropriate value of μ_{sub}/μ_{cut} on the exterior surface.

μ_{cut}	Linear, Eq. (10)	Quadratic, Eq. (21)
1×10^{-6}	0.50004	0.50017
1×10^{-5}	0.50041	0.50170
1×10^{-4}	0.50398	0.51557
1×10^{-3}	0.53275	0.58440
1×10^{-2}	0.61829	0.64986
1×10^{-1}	0.66012	0.64049

The smallest value of μ_{cut} on Fig. 7 is 1×10^{-12}, and no particles scored below this value. As in Sec. 4.1, statistical checks indicated that the tally was well converged even without a grazing approximation. Thus, this is considered the reference total surface flux.

The pink curve on Fig. 7 ("MCNP, 1/2") shows what would happen if a user were limited to the substitute value $\mu_{sub}/\mu_{cut} = \frac{1}{2}$ but if he were able to vary μ_{cut}. He would see the total surface flux changing significantly until some μ_{cut} below 0.01. At some point, the flux would be statistically constant with μ_{cut}, but it is not clear from Fig. 7 where that point is. The fact that different definitions of the grazing range lead to different results indicates a breakdown in the approximation, even without knowing the reference value. [Applying Eq. (20), the error in the integrated flux in the grazing band is 6.5% when $\mu_{cut} = 0.001$. Obviously, the error in the total surface flux is much smaller.]

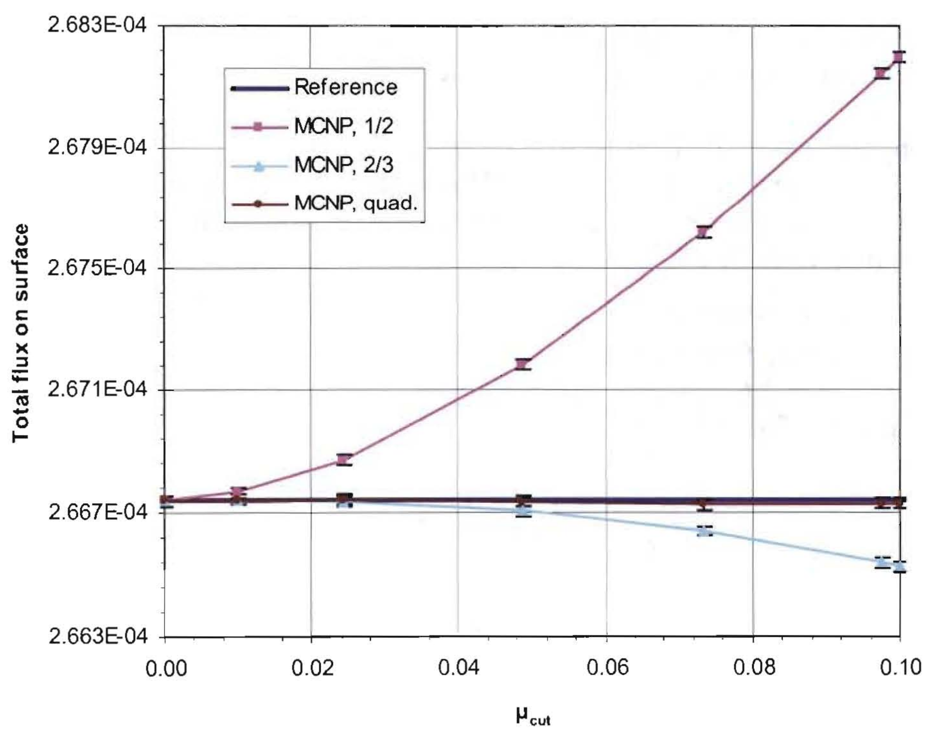

Figure 7. Total flux on the exterior surface as a function of the user-defined grazing angle.

The turquoise curve on Fig. 7 ("MCNP, 2/3") shows that $\mu_{sub}/\mu_{cut} = \frac{2}{3}$ is a much more accurate substitute value than the standard one for large μ_{cut} (> 0.01). Again, however, the curvature indicates a breakdown in the assumptions leading to Eq. (10).

Finally, the dark red curve on Fig. 7 ("MCNP, quad.") is the result that is obtained by applying Eq. (21) for each μ_{cut}. Clearly, this is not possible for realistic problems, but it shows that the correct value of μ_{sub}/μ_{cut} gives the correct grazing flux integral even for very large μ_{cut}.

This problem happens to be one in which grazing fluxes do not pose any difficulties, as evidenced by the fact that the tally needs no grazing-flux approximation at all to succeed. In general, of course, there will be no reference value, grazing fluxes will be troublesome, and it will not be possible to know in advance how the flux varies with the surface-crossing angle cosine. In these cases, analyzing results as a function of μ_{cut} will tell when the assumptions of Sec. 2 are satisfied. When μ_{cut} can be changed without changing a result that *should* be independent of μ_{cut}, then correct values of μ_{sub}/μ_{cut} and μ_{cut} have been found.

Figure 7 provides an argument for allowing both μ_{cut} and μ_{sub}/μ_{cut} to be user inputs in the production codes. The standard value $\mu_{sub}/\mu_{cut} = \frac{1}{2}$ is not appropriate, because the flux is not approximately constant with μ, until very small values of μ_{cut} are used. However, the flux is approximately linear with μ at much larger values of μ_{cut}. The approach suggested in Sec. 3, "always use the standard value $\mu_{sub}/\mu_{cut} = \frac{1}{2}$, but try to set μ_{cut} to a value below which the flux is approximately constant with μ," may be modified in certain situations to "use $\mu_{sub}/\mu_{cut} = \frac{2}{3}$ and try to set μ_{cut} to a value below which the flux is approximately linear with μ."

5. SUMMARY AND CONCLUSIONS

To avoid infinite variances, Monte Carlo surface flux tallies have employed an approximation that has gone unquestioned for decades: for grazing cosines, score the reciprocal of half the grazing-cosine cutoff instead of the reciprocal of the cosine. This approximation was derived assuming that the angular flux is a linear function of the crossing cosine μ. Two further assumptions are also necessary: 1) that the grazing band is symmetric about $\mu = 0$; and 2) that the linear expansion is an accurate representation of the flux in the entire grazing band.

Two simple cases violate these assumptions. One is when users control cosine bins and set up bins that are not symmetric, including the common desire for in-going and out-going fluxes. The other is on an exterior surface, where the flux may be zero for half the range of μ and the linear expansion is not accurate in the entire grazing range, or, to circumvent that difficulty, the range of interest may be limited to the non-zero half-space, violating the first assumption.

In these cases, if the angular flux on the surface is very isotropic, the standard grazing-angle flux approximation applies. If the angular flux on the surface is very linear (with μ), then a different approximation applies: instead of scoring the reciprocal of half the cutoff cosine, score the reciprocal of two-thirds of the cosine cutoff. This paper has shown that if a one-sided flux integral is desired and the angular flux is assumed to be constant in the grazing range but it is in fact linear, the maximum error in the integrated flux in the grazing range is 33%.

In this paper, we have argued that the grazing range cutoff cosine μ_{cut} should be left to the user to determine. He should be able to vary μ_{cut} and see how the results are affected. We have also shown that it would helpful if the substitute value for the grazing range were also left to the user. An appropriate substitute value will allow the user to more easily locate where the response of interest is constant with respect to μ_{cut}.

Some current research has shown the potential to address this problem without the need for approximations based on unverifiable assumptions. Both the ex post facto method [9] and the kernel density estimator [10] may one day be applied to surface flux tallies in production Monte Carlo codes. Until then, users should be given the flexibility to examine these issues themselves.

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